Solubility of Oxygen in Liquid Pyridine

R.D. Mountain[C, S] and P.T. Beaton
National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.

The solubility of oxygen in liquid pyridine is calculated using molecular simulation methods for 300 K and pressures ranging from 0.1 MPa to 10 MPa. The calculated solubilities are compared with experimental results at low pressures. The oxygen molecule is modelled as a rigid object with two Lennard-Jones centers located at the nuclear sites plus a point quadrupole moment located at the center of mass. The Lennard-Jones parameters were developed from a solid-state model and modified so that the equation of state of the fluid is accurately reproduced. The pyridine molecule is modelled as a rigid, all atom object with Lennard-Jones and Coulomb sites located at the nuclear sites (H, C, N). The charges were obtained from quantum chemistry calculations and the Lennard-Jones parameters were taken from the literature and modified so that the experimental density is obtained at 300K and 0.1MPa. The long-range Coulomb interactions are included using the Ewald summation method. The chemical potential of oxygen in the gas phase is obtained by integrating the equation of state and the chemical potential of oxygen in liquid pyridine is obtained by evaluating the insertion charging integral in the NPT ensemble. The sensitivity of the results to the presence of the point quadrupole moment of oxygen is discussed.